CASE BASED MODULE

COMBINED HEATING AND POWER CYCLE FROM WASTE HEAT

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NOMENCLATURE

Symbol / Abbreviation	Description
IEA	International Energy Agency
PC	Power cycle
CHP	Combined heat and power
GWP	Global warming potential
ODP	Ozone depletion potential
ORC	Organic Rankine Cycle
AIT	Auto-ignition temperature
DIPPR	Design Institute for Physical Properties
ATEX	Appareils destinés à être utilisés en ATmosphères EXplosives
GHS	Globally Harmonized System of Classification and Labelling of Chemicals
SP	Size parameter of the fluid
T_{crit}	Critical temperature of the fluid
T_{tp}	Triple point temperature of the fluid
$P_{sat\ @\ T_c}$	Saturated pressure of the fluid at cold temperature
$P_{sat\ @\ T_h}$	Saturated pressure of the fluid at hot temperature
$\rho_{vap\ @\ T_c}$	Vapor density of the fluid at cold temperature
T_{amb}	Ambient temperature
ΔT_{pp}	Pinch point temperature
T_h	Evaporation (hot source) temperature
T_c	Cold temperature
T_u	Thermal utility temperature
f	Fraction of heat input to the output of the utility
η	Efficiency
x	Vapor quality of the fluid
P	Power
ρ	Density of the fluid
h	Enthalpy of the fluid
s	Entropy of the fluid
Q	Heat
V_r	Specific volume ratio of the fluid

ABSTRACT

Since the mid 19th century, thermodynamics principles have enabled the production of work from heat using power cycles. Although effective and popular, one of its major drawbacks is a relatively poor efficiency as most of the heat produced is released into the environment at lower temperatures. Rapidly increasing global energy demands has shifted the focus towards improving the efficiency of our electricity and heating production processes. A potential solution has been found in combined heating and power systems, a subsidiary of power cycles. This technology can use the waste heat that would have otherwise been released into the environment for residential heating and other purposes to augment the overall efficiency of the process. The working fluid used in this cycle plays a major role in its performance. Accordingly, 647 pure fluids from the DIPPR database were subjected to a detailed pre-screening process to identify those that would result in the optimal functionality of both the power and combined heating and power cycle. It considered the thermodynamic suitability (efficiency and the size of the turbine used to produce work), safety and environmental sustainability in its evaluation criteria. An integrated program was developed on MATLAB to perform the screening process as well as to calculate the relevant thermodynamic parameters for the shortlisted fluids. Heat sources characterized by three different temperatures were considered to produce work. In the case of the combined heat and power cycle, the heat used in the thermal utility was categorized into two temperatures, each at two different thermal power fractions from the heat source. The fluids were identified as toxic if they contained certain properties outlined by the GHS. Furthermore, the auto-ignition temperature was used as an appropriate indicator of flammability. The results showed that although around 40% of the total shortlisted fluids were toxic and flammable, many of these fluids also resulted in the most desirable performance characteristics.

INTRODUCTION

According to a recent report by the International Energy Agency (IEA), "global electricity demand is expected to grow by up to 4% in 2022" [1]. This, coupled with the statistic that heating demands account for half of the world's energy consumption [2], the need to make our electricity and heating production processes as efficient as possible, in the most environmentally friendly way to satisfy our societal demands is of the utmost relevance and importance.

Combined heat and power systems represent a key technology that has the potential to achieve this. This technology can convert low-temperature thermal energy sources (geothermal energy, industrial waste heat recovery, solar energy, energy from biomass combustion) into useful work. This system is based on the use of a closed thermodynamic cycle, in which the working fluid in the cycle converts the thermal energy from the heat source into useful work (electricity) by cyclically undergoing thermodynamic transformations in a closed loop. This cycle is known as the power cycle (PC).

Power cycle

There are two main power cycles, the Rankine cycle, and the Brayton cycle. The Rankine cycle is widely used in steam power plants. Its processes use a boiler to generate steam at high pressure and temperature. This steam is expanded in a series of turbines to transform the thermal energy into useful mechanical work to produce electricity. The steam exits from the turbine into a condenser that rejects the unused heat into a heat sink and pumps the low-pressure water back into the boiler to repeat the cycle.

The high temperature required in the evaporator to obtain superheated steam can lead to excessive pressure, creating the risk of erosion of the turbine blades [3]. Several variations of the Rankine cycle have been studied and developed to convert low-temperature heat sources into electricity to increase the overall efficiency of the process and reduce environmental impact. In conventional thermal power generation systems, the part of the thermal energy from the heat source that has not been converted to work is released into the environment which acts as the heat sink. This lost energy reduces the efficiency of the system. Therefore, to optimize the performance of these systems and improve energy efficiency, a part of this released thermal energy is used to meet other heating needs by reconfiguring the conventional Rankine cycle. This is known as the combined heat and power cycle (CHP).

Combined Heat and Power cycle

The CHP cycle operates in the same temperature range as the power cycle but features some changes to the thermodynamic transformations of the working fluid. These changes occur during the expansion of the fluid in the turbine – it exits at temperatures greater than the ambient temperature after expansion in the first turbine and is partially condensed to capture heat. This released heat can be used for heating applications. Next, the fluid continues in the cycle by further expansion in a second turbine to produce more work before it is finally condensed to low pressure and subcooled for re-entry into the boiler to repeat the cycle.

When low-medium grade heat is available (< 400 °C), CHP can employ an organic Rankine cycle to exploit these heat sources for electricity generation. The Organic Rankine Cycle (ORCs) has the same physical configuration as the traditional cycle but operates with organic fluids that have a boiling temperature below that of water. It can also operate with a variety of hot sources, like geothermal and solar energy, and industrial waste heat [4], making it an attractive solution to problems created by the traditional cycle.

Selection of fluids

The selection of appropriate working fluids is critical in the design of an efficient CHP cycle. It depends on several factors, related to thermodynamic properties of the fluid or to the operating characteristics of the cycle. For example, in the most recent applications, suitable fluids should have low viscosity and specific volume, work in moderate pressures in heat exchangers and have a low global warming potential (GWP), ozone depletion potential (ODP), toxicity and inflammability [2].

In the past two decades, research has been focused on the development of precise fluid screening processes for low temperature applications. Papadopoulos et al. presented a first approach of fluid selection for ORCs in 2009, using a computational tool named computer aided molecular design (CAMD) and process optimization methods. This study concluded that using arbitrary fluid databases can potentially limit the identification of the most efficient possibilities [5]. In 2013, Bao and Zhao worked closely with parameters to be considered for screening pure fluids and mixtures such as vaporization latent heat, specific heat, boiling point, molecular weight. It was concluded that although the parameters analyzed could be sufficient for the screening of pure fluids, more advanced research needed to be considered for mixtures [3].

Shu et al. published a study in 2017 that analyzed the dynamic response of 14 ORCs using a dynamic model on Simulink. Parameters such as rise time, settling time and time constant were compared. Each system worked with a different working fluid. using waste heat from internal combustion engines as the heat source. The results showed that time response for low temperature working fluids was usually faster than high temperature working fluids so a traditional Rankine cycle would respond slower than an organic one [6].

Zhao et al. presented a model for the optimization of working fluids and cycle parameters in ORC at the molecular scale in 2017, based on the proper cycle parameters and safety and environmental analysis. It solved some limitations of previous research such as restricted datasets that only presented conventional molecules and focused mainly on properties of the fluid. By developing this new model for molecular design and cycle optimization, it was concluded that both parameters can be optimized simultaneously [7].

In 2021, Lasala et al. presented a methodology for the selection of promising working fluids for combined cooling, heat, and power (CCHP) applications. The screening considered thermodynamic properties as well as safety, environmental, constructional, and process-related limitations. Moreover, the Peng-Robinson cubic equation of state was applied to ensure the precision of the calculation of the thermophysical properties. The results following a database search and screening of about 60,000 fluids indicated that flammable fluids have a favorable potential to serve as a working fluid in CCHP applications [2].

Safety

Toxicity and flammability are the primary determinants of safety in this case. Firstly, a toxicity screening indicates the suitability of the working fluids for domestic or industrial use. Suitable fluids that are carcinogenic, mutagenic, acutely toxic to humans, toxic to specific human organs, or cause harmful reproductive effects are considered with caution [2]. The classification was adopted using a set of codes from the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) [8]. Secondly, the auto-ignition temperature (AIT) is used as an appropriate indicator of flammability by considering the maximum surface temperature of a system according to the ATEX directive [9].

Size parameter

The performance of the power and CHP cycle configurations is determined through the analysis of a non-dimensional quantity called the size parameter. In this study, the primary indicator was the size of the turbine. This is because the size of a Rankine cycle strongly depends on this parameter, as it increases with increasing expansion ratio. The size of a turbine is defined by its specific volume ratio – the variation of specific volume across the turbine in a real process ($V_r = V_{out}/V_{in}$).

Alternatively, other equations are presented in the literature and are used to obtain the size parameter of a turbine in power cycles. In processes where the thermal energy of the source is quantitatively defined, the mass flow of the working fluid can be obtained. It is common to calculate the size parameter as a relation between the volumetric flow rate at the outlet of the turbine and the isentropic variation of enthalpy in the turbine's expansion process $\left(SP = V_{out}^{0.5}/\Delta h_{ise}^{0.25}\right)$. The dimension of this size parameter is *meters* [10].

In the above case, an analysis of the cycle efficiency is performed using the values of the SP and the isentropic volumetric flow rate relation of the turbine $\left(V_{r,ise} = V_{out,ise}/V_{in}\right)$. It is understood that the maximum attainable efficiency from a single stage ORC turbine is a decreasing function of volume ratio $V_{r,ise}$. This implies that high values for $V_{r,ise}$ will lead to poor efficiency due to the presence of big flaring angles, supersonic flows, and high kinetic losses. Consequently, it might be preferable to consider adopting multi-point turbines to split the expansion into two or more points. However, the benefits of adopting a higher number of turbine points are constrained by the inflated cost of components and higher cost of energy required for its operation [10].

Objective of the project

The aim of this project was to identify pure working fluids that would optimize the performance of the power and CHP cycles with respect to the size of key cycle components, environmental, safety (toxicity and flammability) and operating constraints. 647 pure fluids extracted from the Design Institute for Physical Properties (DIPPR) database were considered in this study. Heat sources characterized by three different temperatures were considered to produce work. In the case of CHP, the heat used in the thermal utility was categorized into two temperatures, each at two different thermal power fractions from the heat source.

METHODOLOGY

Working fluid screening process

The criteria on which the 647 fluids were screened to identify the most suitable ones is shown in Table 1.

Table 1: Summary of pre-screening criteria

#	Parameter	Abbreviation	Selection Criteria
1	Critical temperature	T_{crit}	$> T_{evap} + 5℃$
2	Triple point temperature	T_{tp}	$< T_{amb}$
3	Saturation pressure at cold temperature	$P_{sat\ @\ T_c}$	> 1 bar at T_c: $T_{evap} = 150℃$
			> 100 mbar at T_c: $T_{evap} = 250℃$
			> 5 mbar at T_c: $T_{evap} = 350℃$
4	Saturation pressure at hot temperature	$P_{sat\ @\ T_h}$	< 35 bar at T_h: $T_{evap} = 150℃$
			< 70 bar at T_h: $T_{evap} = 250℃$
			< 150 bar at T_h: $T_{evap} = 350℃$
5	Density at cold temperature	$\rho_{vap\ @\ T_c}$	$> 0.01 \frac{kg}{m^3}$
6	Global Warming Potential	GWP	< 150
7	Ozone Depletion Potential	ODP	Exclude molecules containing Br
8	Auto-ignition temperature	AITC	$\frac{T_{evap}}{0.8}$

Table 2 explains the selection of each pre-screening criteria and its values (where applicable).

Table 2: Explanation for pre-screening criteria and its values

#	Parameter	Explanation of criteria	Explanation of selected values
1	T_{crit}	Ensure sufficiently high enthalpy of vaporization and that the fluid in the cycle is in the subcritical range	Existence of ORC in two-phase region and to allow a margin to make criteria less rigid
2	T_{tp}	Ensure the fluid in the cycle does not solidify at the minimum cycle temperature	Desirable to be lower than the minimum temperature of the cycle
3	$P_{sat@\ T_c}$	Limit inverse pressure gradient to avoid entry of air at the lowest pressure point of the cycle	Experimental minimum pressure according to Preißinger et al. [11]
4	$P_{sat\ @\ T_h}$	Prevent mechanical failure of the turbine due to excessive pressure	Experimental maximum pressure according to Quoilin et al. [12]
5	$\rho_{vap\ @\ T_c}$	Ensure adequately low cross-section of the condenser tubes – the lower the density, the larger the area	Suggested minimum saturated vapor density according to Quoilin et al. [12]
6	GWP	Scientific Assessment of Ozone Regulation [13]	EU F-gas regulation [14]
7	ODP		EU regulation No. 1005/2009 [15]
8	AIT	Maximum surface temperature of the system must not exceed 80% of the auto-ignition temperature of the substance [9]	

Process diagram: Working fluid screening & computation of cycle parameters

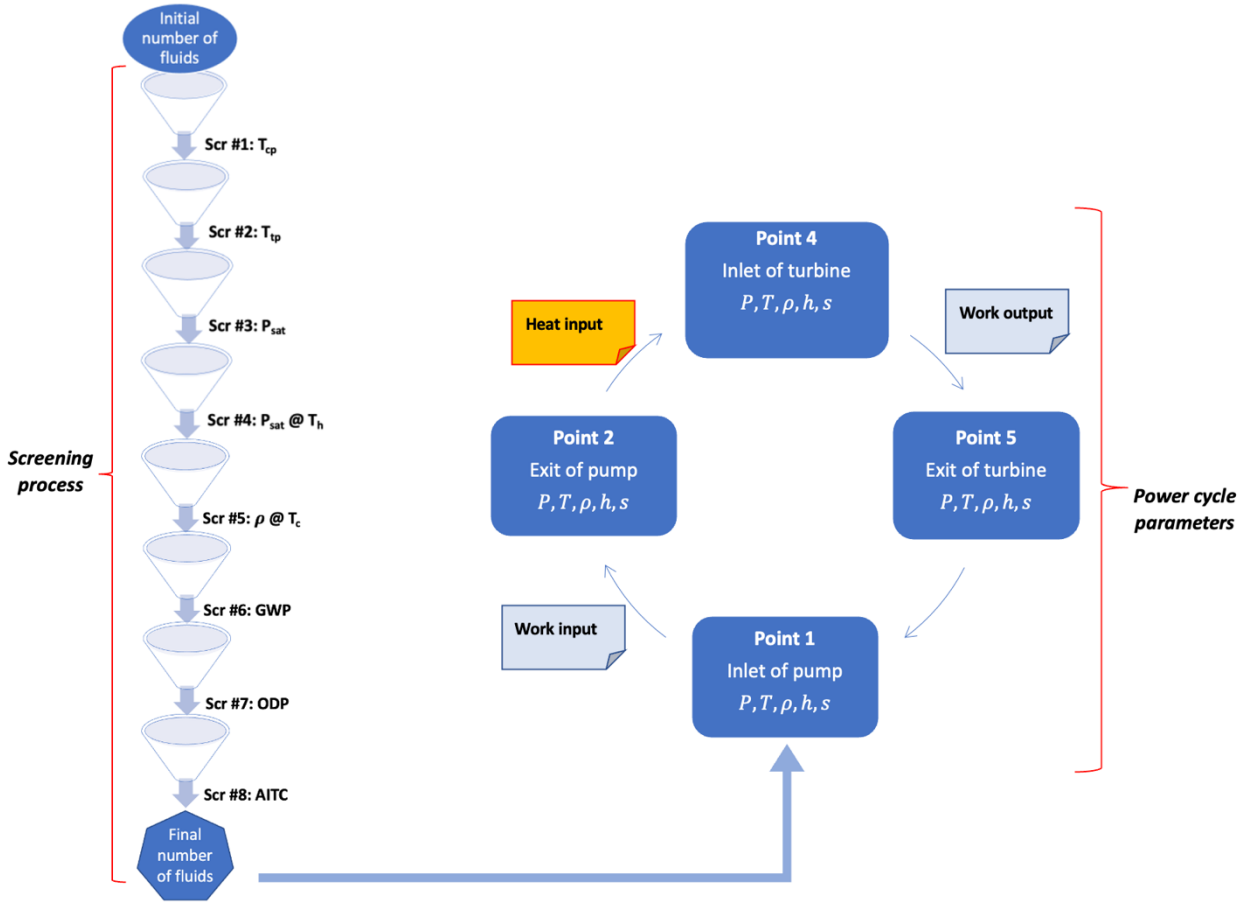

Figure 1: Process diagram for the power cycle

The process diagrams shown in Figure 1 and Figure 2 represent the overall pre-screening and calculation process adopted in the case of the power and CHP cycles. Following the identification of the most desirable working fluids using the 8 different screening criteria, the most relevant parameters (pressure, temperature, density, enthalpy, and entropy) at each point of the cycles were determined for each of the working fluids. The general calculation procedure is shown subsequently in the *Calculation methodology* section for both cycles. Once the net power, thermal utility heat, and efficiency of the cycle were calculated for each fluid, a validation step was done to determine which fluids were toxic as shown in the *Toxicity screening* section.

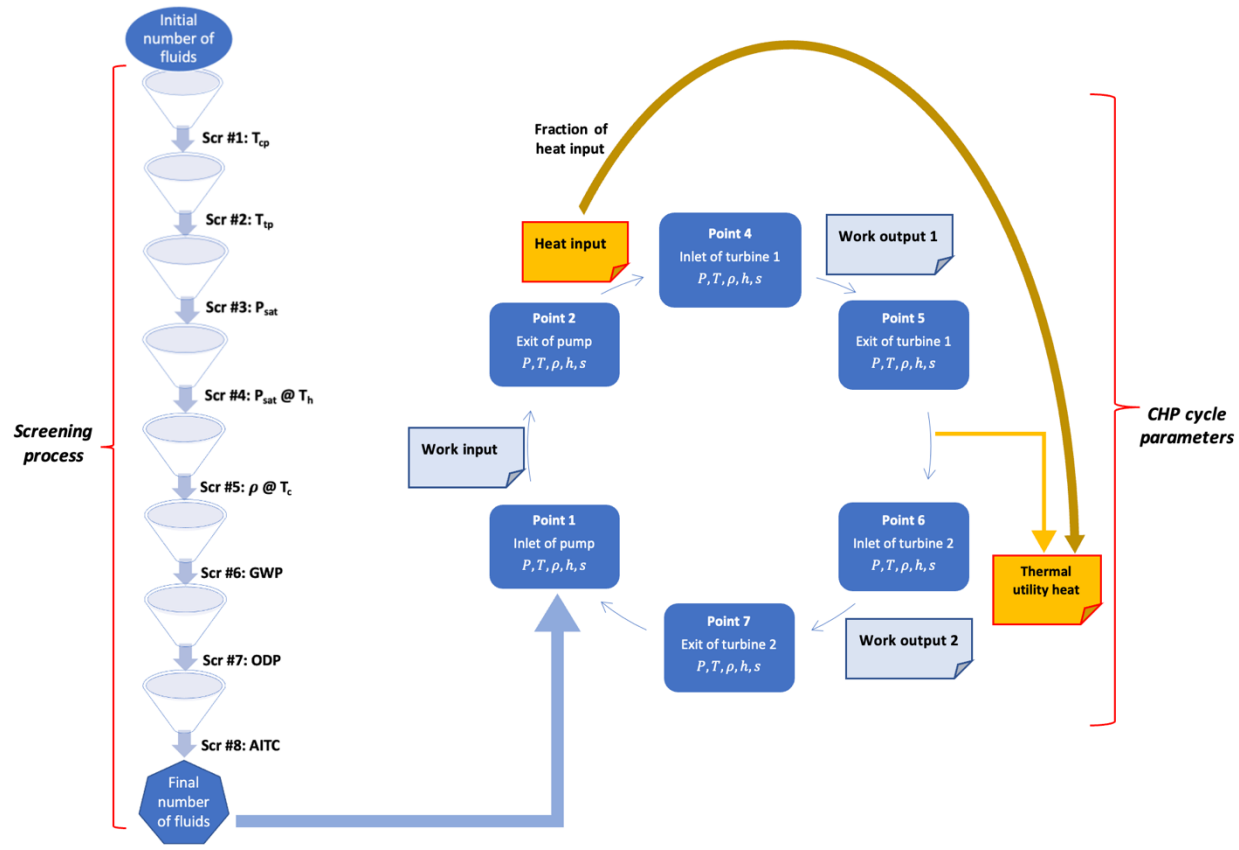

Figure 2: Process diagram for the CHP cycle

Functionality of *Thermoprop*

An accurate and efficient way to determine the relevant working fluid parameters for pure fluids, such as temperature, pressure, density, vapor quality, enthalpy, and entropy is by using a program known as *Thermoprop*. Developed by the *"Thermodynamique et Energie"* team of the *Centre National de la Recherche Scientifique* (CNRS), it is based on the Peng-Robinson cubic equation of state for pure fluids currently available [2]. Its functionality requires the knowledge of two independent intensive phase variables for a given working fluid to directly determine the unknown variables. Although built independently, *Thermoprop* is accessible through MATLAB. The figure below explains the *Thermoprop* function in the above context.

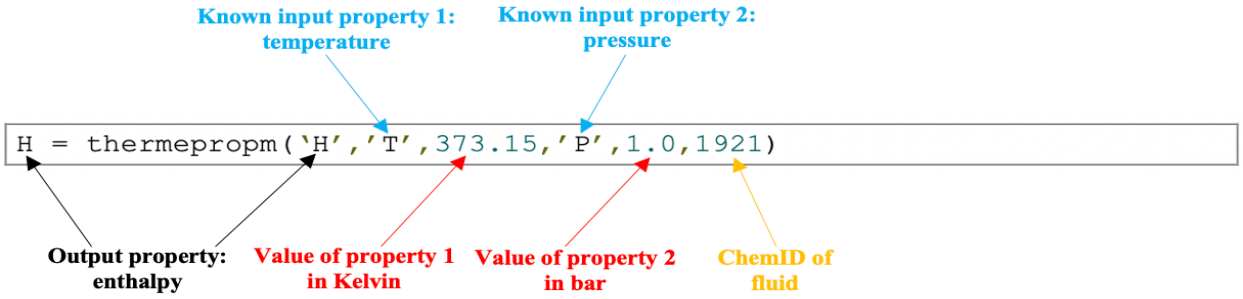

Figure 3: Functionality and syntax of Thermoprop

As shown in Figure 3, *Thermoprop* is used to find the enthalpy of a working fluid with ChemID 1921, which corresponds to water. The ChemID is a unique identification number assigned to each fluid under analysis. The input pair of properties in this case are temperature and pressure.

Calculation methodology

Table 3 lists the predefined conditions that would be relevant when computing the operational parameters of the power and CHP cycles. Note that the highlighted parameters are only applicable to the CHP cycle, while the others apply to both the power and CHP cycles.

Table 3: Summary of design constraints and parameters

Parameter	Abbreviation	Unit	Value
Ambient temperature	T_{amb}	℃	20
Pinch point temperature	ΔT_{pp}	℃	10
Evaporation temperature	T_h	℃	150
			250
			350
Thermal utility temperature	T_u	℃	40
			80
Fraction of heat input to the output of the utility	f	%	10
			40
Pump efficiency	η_{pump}	-	1.00
Turbine efficiency	$\eta_{turbine}$	-	0.85
Desired minimum vapor quality at turbine outlet	$x_{turb,2}$	-	0.60[1]

[1] This criteria is not strictly imposed for the rejection of fluids, considering new research on the development of turbines able to work with two-phase fluids [19].

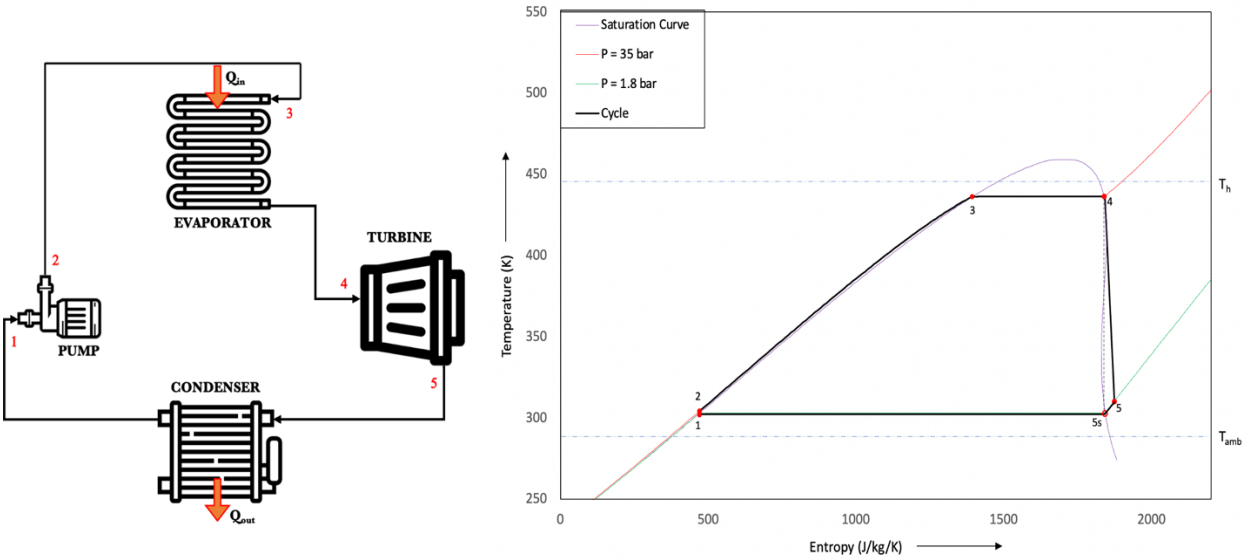

Figure 4: T-s diagram for cyclobutane and schematic of the power cycle

Figure 4 shows the T-s diagram (to scale) for the **power cycle.** The computations below have been performed in the same order as the points shown in the diagram.

The first step is to determine the temperature at the inlet of the pump (at *Point 1*) – the lowest temperature of the cycle. This is also referred to as the cold temperature T_c. The temperature at this point must be greater than the ambient temperature to ensure heat transfer between the working fluid and ambient air.

$$T_1 = T_{amb} + \Delta T_{pp} \tag{1}$$

The pressure at *Point 1* can be determined from *Thermoprop* as it is the saturation pressure at T_1.

$$P_1 = P_{sat\ @\ T_1} \tag{2}$$

Now, two independent intensive phase variables are known, so the remaining properties at *Point 1*, density, enthalpy, and entropy, can be determined from *Thermoprop*.

To determine the properties at the exit of the pump, this is divided into two points – *Point 2s*, which corresponds to the ideal (isentropic) case and *Point 2*, which corresponds to the real case. First, it is necessary to proceed momentarily to *Point 4* – the inlet of the turbine. This is because two parameters are already known at this point:

1. The evaporation temperature T_h.
2. At the inlet of turbine, the fluid is heated at constant pressure until it forms a saturated vapor, so the vapor quality x is 1.

$$P_4 = P_{sat\ @\ T_h\ \&\ x\,=\,1} \tag{3}$$

As the heat addition is done at constant pressure, the properties at *Point 2s* can effectively be determined as shown below.

$$P_4 = P_{2s} \tag{4}$$

$$s_{2s} = s_1 \tag{5}$$

The remaining properties, temperature, density, and enthalpy can be determined from *Thermoprop*.

Given that the isentropic efficiency of the pump η_{pump} is known, the properties at *Point 2* can also be determined using Equations (6-8).

$$\eta_{pump} = \frac{h_{2s} - h_1}{h_2 - h_1} \tag{6}$$

$$h_2 = h_1 + \frac{h_{2s} - h_1}{\eta_{pump}} \tag{7}$$

$$P_2 = P_{2s} \tag{8}$$

The remaining properties, temperature, density, and entropy can be determined from *Thermoprop*.

Returning to *Point 4*, the properties at this point can now be determined as well.

$$P_4 = P_{sat\ @\ T_h\ \&\ x\,=\,1} \tag{9}$$

$$T_4 = T_h \tag{10}$$

The remaining properties, density, enthalpy, and entropy can be determined from *Thermoprop*.

The exit of the turbine can also be divided into 2 points - *Point 5s,* which corresponds to the ideal (isentropic) case and *Point 5*, which corresponds to the real case. In both cases, the pressure corresponds to the condenser pressure, so the properties at *Point 5s* can be determined.

$$P_{5s} = P_1 \tag{11}$$

$$s_{5s} = s_4 \tag{12}$$

The remaining properties, temperature, density, and enthalpy can be determined from *Thermoprop*.

Lastly, given that the isentropic efficiency of the turbine $\eta_{turbine}$ is known, the properties at *Point 5* can also be determined using Equations (13-15).

$$\eta_{turbine} = \frac{h_4 - h_5}{h_4 - h_{5s}} \tag{13}$$

$$h_5 = h_4 - \eta_{turbine}(h_4 - h_{5s}) \tag{14}$$

$$P_5 = P_{5s} \tag{15}$$

The remaining properties, temperature, density, and entropy can be determined from *Thermoprop*.

The calculation of these properties will allow the net power (P_{net}), heat input (Q_{in}), and efficiency of the power cycle (η_{cycle}) to be determined. Note that all the parameters have been calculated on a **per unit mass flow rate basis** as the actual mass flow rate of the working fluid is unknown.

$$P_{turbine} = h_4 - h_5 \tag{16}$$

$$P_{pump} = h_2 - h_1 \tag{17}$$

$$P_{net} = P_{turbine} - P_{pump} \tag{18}$$

$$Q_{in} = h_4 - h_2 \tag{19}$$

$$\eta_{cycle} = \frac{P_{net}}{Q_{in}} \tag{20}$$

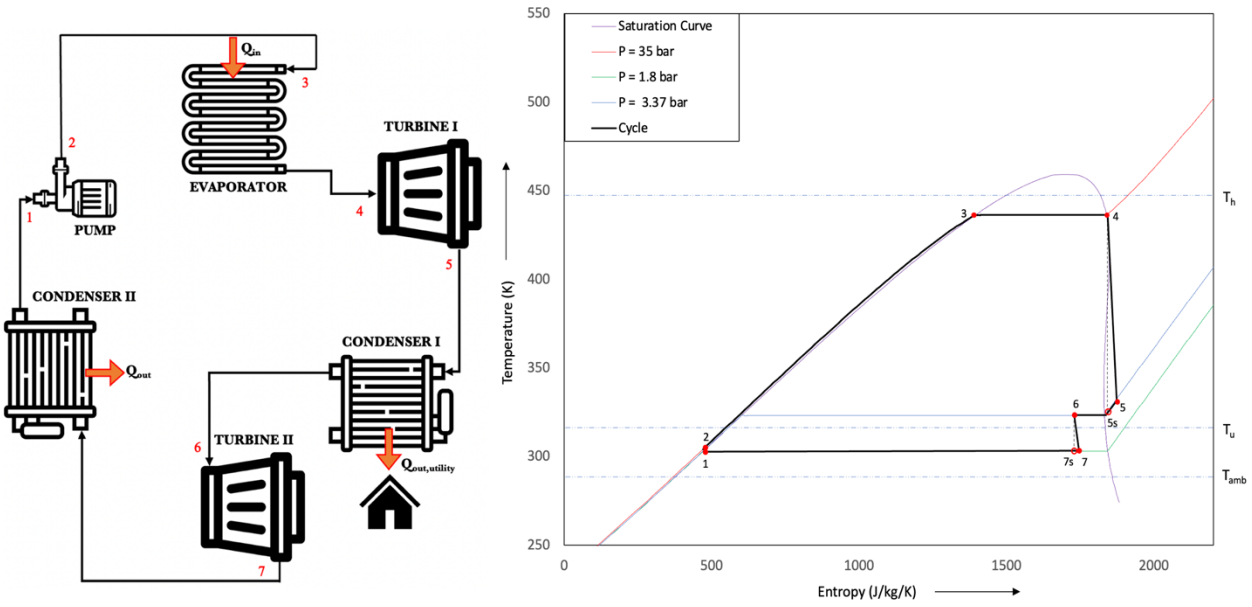

Figure 5: T-s diagram for cyclobutane and schematic of the CHP cycle

Figure 5 shows the T-s diagram for the **CHP cycle.** The computations below have been performed in the same order as the points shown in the diagram.

The calculation procedure for Points 1, 2 and 4 are the same as in the power cycle. Therefore, these steps will not be repeated here.

Starting from the exit of turbine 1, this can be divided into 2 points - *Point 5s,* which corresponds to the ideal (isentropic) case and *Point 5*, which corresponds to the real case. The pressure is the saturation pressure at the sum of the utility and pinch point temperatures. This can therefore be determined directly from *Thermoprop*.

$$T = T_u + \Delta T_{pp} \tag{21}$$

$$P_{5s} = P_{sat\ @\ T_u + \Delta T_{pp}} \tag{22}$$

$$s_{5s} = s_4 \tag{23}$$

Given the knowledge of two independent intensive phase variables, the remaining properties, temperature, density, and enthalpy can be found directly from *Thermoprop*.

The isentropic efficiency of turbine 1 $\eta_{turbine,1}$ is known, so the properties at *Point 5* can be determined using Equations (24-26).

$$\eta_{turbine,1} = \eta_{turbine} = \frac{h_4 - h_5}{h_4 - h_{5s}} \tag{24}$$

$$h_5 = h_4 - \eta_{turbine}(h_4 - h_{5s}) \tag{25}$$

$$P_5 = P_{5s} \tag{26}$$

The remaining properties, temperature, density, and entropy can be determined from *Thermoprop*.

Point 6 represents the inlet of turbine 2. In this case, the enthalpy can be determined directly using Equations (27-28) as it is a function of the fraction of heat *f* supplied into the utility.

$$h_6 = h_5 - f(h_4 - h_2) \tag{27}$$

$$P_6 = P_5 \tag{28}$$

The remaining properties, temperature, density, and entropy are directly available using *Thermoprop*.

It is also necessary to verify if the vapor quality at the inlet of turbine 2 meets the desired minimum level stated in Table 3. This can also be done using *Thermoprop*.

The exit of turbine 2 can be divided into two points – *Point 7s* which corresponds to the ideal (isentropic) case and *Point 7*, which corresponds to the real case. Examining the ideal case first:

$$P_{7s} = P_1 \tag{29}$$

$$s_{7s} = s_6 \tag{30}$$

The remaining properties, temperature, density, and enthalpy can be determined from *Thermoprop*.

Finally, the isentropic efficiency of turbine 2 $\eta_{turbine,2}$ is known, so the properties at *Point 7* can be determined using Equations (31-33).

$$\eta_{turbine,2} = \eta_{turbine} = \frac{h_6 - h_7}{h_6 - h_{7s}} \tag{31}$$

$$h_7 = h_6 - \eta_{turbine}(h_6 - h_{7s}) \tag{32}$$

$$P_7 = P_{7s} \tag{33}$$

The remaining properties, temperature, density, and entropy can be determined from *Thermoprop*.

The calculation of these properties will allow the net power (P_{net}), heat input (Q_{in}), heat for the thermal utility (Q_u) and efficiency of the CHP cycle (η_{cycle}) to be determined. Note that all the parameters have been calculated on a **per unit mass flow rate basis** as the actual mass flow rate of the working fluid is unknown.

$$P_{turbine,1} = h_4 - h_5 \tag{34}$$

$$P_{turbine,2} = h_6 - h_7 \tag{35}$$

$$P_{pump} = h_2 - h_1 \tag{36}$$

$$P_{net} = P_{turbine,1} + P_{turbine,2} - P_{pump} \tag{37}$$

$$Q_{in} = h_4 - h_2 \tag{38}$$

$$Q_u = f Q_{in} \tag{39}$$

$$\eta_{cycle} = \frac{P_{net} + Q_u}{Q_{in}} \tag{40}$$

Toxicity screening

Fluids containing the GHS toxicity codes shown in Table 4 were flagged as toxic.

Table 4: Toxicity screening categories

Parameter	Toxicity categories to be flagged
Toxicity	H305, H310, H314, H318, H330, H331, H334, H340, H341, H350, H351, H360, H361, H362, H370, H372, H373

Size parameter

The specific volume ratio $V_r = \frac{V_{out}}{V_{in}}$ is the indicator adopted to determine the optimal working fluid for each power and CHP cycle configuration. This analysis was done on a plot of cycle efficiency (η_{cycle}) against its specific volume ratio. For the power cycle, specific volume ratio was calculated by dividing specific volume at *Point 5* by specific volume at *Point 4*. For the CHP cycle, it is the ratio of the specific volume at *Point 7* (outlet of the second turbine) to the specific volume at *Point 4* (inlet of the first turbine).

RESULTS AND DISCUSSION

Table 5: Number of fluids after each successive screening step

Screening step	Screening parameter	No. of fluids for $T_h = 150$ ℃	No. of fluids for $T_h = 250$ ℃	No. of fluids for $T_h = 350$ ℃
0	Initial count	647	647	647
1	T_{crit}	589	466	216
2	T_{tp}	522	399	151
3	$P_{sat\ @\ T_c}$	29	52	23
4	$P_{sat\ @\ T_h}$	20	52	21
5	$\rho_{vap\ @\ T_c}$	20	52	21
6	GWP	18	50	21
7	ODP	18	49	20
8	AITC	18	35	15

Table 5 shows the results for the number of fluids that remained following each step of the screening process, for the three different evaporation temperatures. These results show that the third step screened out the highest number of fluids at evaporator temperatures of 150 ℃ and 250 ℃, whereas the first step rejected the highest number of fluids at 350 ℃. It is also evident that the saturation pressure at the hot source temperature and vapor density had the least effect. The number of fluids at 250 ℃ is significantly greater than at both 150 ℃ and 350 ℃. This suggests that there is a greater likelihood of extracting more suitable fluids at 250 ℃ than at the other two temperatures. It must be reiterated that these results also include toxic fluids as the toxicity screening has not been carried out at this point. The complete list of fluids for each of the evaporation temperatures is given in ANNEX 1: Performance summary.

It can be observed from ANNEX 1: Performance summary that fluids like *cyclobutane*, *vinylacetylene*, *ethyl chloride*[*], *dichlorofluoromethane*[*] showed promising results for an evaporation temperature of 150 °C, higher range of efficiency with a small size parameter. Among these fluids, *ethyl chloride* and *dichlorofluoromethane* are toxic. *Dichlorofluoromethane* (R-12) was previously used as a refrigerant but has been banned in several countries due to its damaging effects on the ozone layer [16]. *Ethyl chloride*[*] and *vinylacetylene* are extremely flammable fluids. Availability, supply, and synthesis process of the fluids also need to be considered for its use in a power or CHP cycle.

Cis-1,2-dicholorethylene[*], *methyl iodide*[*], *isopropyl iodide*, *thiophene*[*] are some fluids with higher efficiencies and lower size parameters at an evaporation temperature of 250 °C. *Cis-1,2-dichloroethylene*[*], *isopropyl iodide* and *thiophene*[*] are flammable. *Thiophene*[*] is acutely toxic, corrosive and irritant. Given that the condenser pressure is lower than the atmospheric pressure at this evaporation temperature, it induces air inflow into the cycle through leakages so the cost of equipment to prevent this will be higher.

[*] Toxic fluids

Interestingly, *Thiophene*[*] has been claimed to produce higher efficiencies and lower system costs than steam or other power cycle working fluids for applications with an evaporation temperature below 750 °F, and power outputs of 5,000 horsepower or less. The principal advantage of this fluid is in its ability to use compact, single stage axial or radial flow turbines which can be less costly per shaft horsepower than multistage steam turbines (US Patent 3,292,366) [17].

Ethynylbenzene[*], *pyrrole*, *tetrahydrothiophene*, *arsenic (III) chloride* are among the few promising fluids at an evaporation temperature of 350 °C. *Ethynylbenzene*[*] is an aromatic hydrocarbon used as a petroleum additive. High level exposure to airborne *ethylbenzene* may lead to health hazards and is also flammable. *Tetrahydrothiophene* is flammable and has been used as an odorant in LPG and natural gas. *Arsenic (III) chloride* is a corrosive, acutely toxic, health and environmentally hazardous fluid. The condenser pressure at an evaporation temperature of 350 °C is significantly below atmospheric pressure so the injection of air into the system will increase the cost of equipment [18].

Overall, the fluids showing the most promising results are flammable while several show toxic characteristics as well. This makes the selection of fluids more complicated.

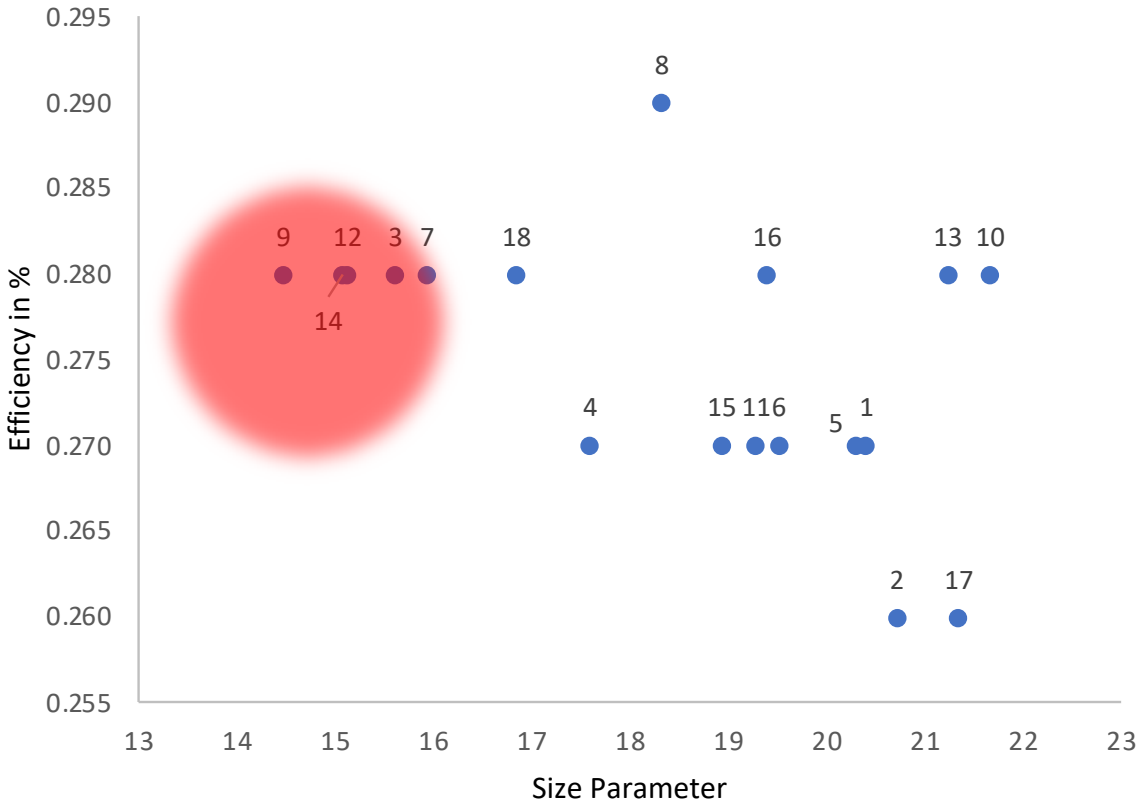

Figure 6: Efficiency vs size parameter plot for T_h=150℃, T_u=40℃, f=0.1

[*] Toxic fluids

Figure 6 shows the plot of cycle efficiency versus size parameter at an evaporator temperature of 150 ℃ and thermal utility temperature of 40 ℃ with 10% of heat input used in the output of the utility. The most desirable fluids are those that result in the highest cycle efficiency with the smallest size parameters. This is indicated by the cluster marked in red at the top left of the figure. The toxicity screening revealed that the fluids marked *12* and *14* were toxic, so the only safe choices were *3* and *9 – cyclobutane and vinylacetylene* respectively. It can also be argued that fluid *8* is suitable as it leads to a higher efficiency, but the size parameter in this case is greater. Overall, these results are testament to the potential compromise that must be reached between cycle efficiency and size parameter. A fluid that can produce a very high efficiency will most likely require a large turbine, and vice versa. If more than one fluid has the suitable characteristics, they can be analyzed closely to identify whether it is advisable to make a compromise on the efficiency or the size parameter.

ANNEX 2: Efficiency versus Size Parameter plots demonstrate that the optimal fluids remain the same for each case irrespective of the thermal utility temperature and thermal power fraction at the respective evaporator temperatures. This observation is consistent for both the power and CHP cycles. This general trend can be validated by means of calculation to show that the optimal fluids for most of these cases will be the same in both cycles.

A separate remark needs to be made on the quality of the fluid at the inlet of the second turbine. Given the recent availability of modern turbines that can work efficiently and durably in the two-phase region [19], fluids with vapor qualities less than 0.6 as stated in Table 3 were also considered in the final shortlist of fluids. However, this may not be the case depending on the type of turbine. For instance, if a more traditional turbine that does not allow the use of two-phase fluids is used, the overall screening process would need to be modified to exclude fluids that would operate in the two-phase region.

CONCLUSION

The results demonstrate the presence of several optimal fluids for each case at all the different evaporator temperatures. Increasing the evaporator temperature increases the efficiency of the power cycle at constant ambient temperature. Moreover, no single fluid is ideal for every case – the decision on the optimal fluid depends on the other conditions of the power plant. From a thermodynamics perspective, the size parameter increases with the increase in evaporator temperature because there is greater expansion in the turbine.

Potential improvements to this project can be made by taking the cost of fluids as well as that of the overall system into account. Additionally, the accuracy of the results could be improved by performing the calculations for an actual cycle with reheating, superheating, and feedwater heating.

This study shows clear evidence that the importance of the choice of the appropriate working fluid in both power and CHP cycles cannot be understated. The selection of the most relevant thermodynamic screening parameters as well as those that influence the safety and environmental sustainability all require in-depth research. Although priority needs to be allocated to the fluids that can best optimize the performance of each cycle, particular emphasis needs to be placed on their cost and potential environmental impact.

ANNEX 1: Performance summary

Evaporation Temperature at 150 °C			POWER CYCLE		COMBINED HEAT AND POWER CYCLE							
					Thermal Utility Temperature = 40 ºC				Thermal Utility Temperature = 80 °C			
					10% Q_{in}		40% Q_{in}		10% Q_{in}		40% Q_{in}	
S.No	**CHEM ID**	**Fluid Name**	**η**	**V_r**	**η**	**V_r**	**η**	**V_r**	**η**	**V_r**	**η**	**V_r**
1	8	ISOPENTANE	0.17	21.16	0.27	19.91	0.55	12.56	0.26	20.01	0.52	13.42
2	9	NEOPENTANE	0.16	21.40	0.26	20.22	0.54	13.03	0.25	20.31	0.51	13.90
3	**102**	**CYCLOBUTANE**	**0.19**	**16.43**	**0.28**	**15.12**	**0.57**	**9.17**	**0.28**	**15.29**	**0.53**	**9.89**
4	205	cis-2-BUTENE	0.17	18.57	0.27	17.10	0.55	10.52	0.26	17.29	0.52	11.32
5	209	1-PENTENE	0.18	21.19	0.27	19.81	0.56	12.20	0.27	19.94	0.53	13.09
6	213	3-METHYL-1-BUTENE	0.17	20.21	0.27	19.02	0.55	12.01	0.26	19.12	0.52	12.84
7	302	1,2-BUTADIENE	0.18	16.78	0.28	15.44	0.56	9.42	0.27	15.61	0.53	10.15
8	404	DIMETHYLACETYLENE	0.19	19.37	0.29	17.83	0.57	10.77	0.28	18.04	0.53	11.63
9	**418**	**VINYLACETYLENE**	**0.18**	**15.18**	**0.28**	**13.98**	**0.56**	**8.53**	**0.27**	**14.14**	**0.53**	**9.19**
10	419	3-METHYL-1-BUTYNE	0.18	22.78	0.28	21.17	0.56	12.90	0.27	21.35	0.53	13.87
11	1407	METHYL ETHYL ETHER	0.17	20.37	0.27	18.79	0.55	11.54	0.26	18.99	0.52	12.42
12	**1503**	**ETHYL CHLORIDE***	**0.19**	**15.89**	**0.28**	**14.63**	**0.57**	**8.86**	**0.28**	**14.80**	**0.53**	**9.56**
13	1694	2,2-DICHLORO-1,1,1-TRIFLUOROETHANE*	0.18	22.40	0.28	20.74	0.56	12.64	0.27	20.95	0.53	13.61
14	**1696**	**DICHLOROFLUOROMETHANE***	**0.19**	**15.82**	**0.28**	**14.58**	**0.57**	**8.85**	**0.27**	**14.74**	**0.53**	**9.55**
15	1703	TRIMETHYLAMINE*	0.17	19.95	0.27	18.44	0.55	11.36	0.26	18.64	0.52	12.22
16	1704	ETHYLAMINE*	0.18	20.54	0.28	18.90	0.56	11.48	0.27	19.12	0.53	12.39
17	1984	TETRAMETHYLSILANE	0.16	22.01	0.26	20.85	0.54	13.81	0.25	20.93	0.51	14.68
18	2642	1,2-DIFLUOROETHANE	0.18	17.76	0.28	16.35	0.56	9.96	0.27	16.53	0.53	10.74

* Fluid is toxic. Special care needs to be taken in the selection of such fluids, if chosen for application.

Evaporation Temperature at 250 °C			POWER CYCLE		COMBINED HEAT AND POWER CYCLE							
					Thermal Utility Temperature = 40 °C				Thermal Utility Temperature = 80 °C			
					10% Q_{in}		40% Q_{in}		10% Q_{in}		40% Q_{in}	
S.No	CHEM ID	Fluid Name	η	V_r	η	V_r	η	V_r	η	V_r	η	V_r
1	22	2,3-DIMETHYLPENTANE	0.21	329.00	0.31	312.41	0.60	209.53	0.30	313.37	0.57	220.48
2	24	3,3-DIMETHYLPENTANE	0.20	289.12	0.30	274.96	0.59	190.29	0.30	275.73	0.57	199.49
3	25	2,2,3-TRIMETHYLBUTANE	0.20	276.70	0.30	263.23	0.59	182.90	0.30	263.95	0.57	191.70
4	105	METHYLCYCLOPENTANE	0.23	234.52	0.33	220.34	0.62	129.74	0.33	221.57	0.59	139.25
5	108	1,1-DIMETHYLCYCLOPENTANE	0.22	276.10	0.32	261.13	0.61	162.43	0.32	262.18	0.59	172.61
6	110	trans-1,2-DIMETHYLCYCLOPENTANE*	0.23	293.11	0.32	276.98	0.61	171.07	0.32	278.14	0.59	181.96
7	111	cis-1,3-DIMETHYLCYCLOPENTANE	0.23	290.75	0.32	274.83	0.61	170.03	0.32	275.96	0.59	180.82
8	112	trans-1,3-DIMETHYLCYCLOPENTANE	0.23	282.34	0.32	266.94	0.61	165.48	0.32	268.03	0.59	175.92
9	226	4-METHYL-1-HEXENE	0.22	342.23	0.31	323.88	0.60	207.66	0.31	325.10	0.58	220.06
10	233	2-ETHYL-1-PENTENE	0.22	317.21	0.32	300.75	0.61	194.85	0.31	301.81	0.58	206.21
11	239	3-ETHYL-1-PENTENE*	0.21	351.63	0.31	332.79	0.60	213.25	0.31	334.04	0.57	225.97
12	248	2,3,3-TRIMETHYL-1-BUTENE	0.20	270.80	0.30	256.96	0.59	172.29	0.30	257.78	0.57	181.40
13	286	1-METHYLCYCLOPENTENE	0.24	225.02	0.34	209.74	0.63	119.10	0.34	211.32	0.60	128.78
14	314	trans,trans-2,4-HEXADIENE*	0.23	292.55	0.33	274.41	0.62	161.29	0.33	276.02	0.59	173.39
15	501	BENZENE*	0.26	198.22	0.36	181.26	0.64	100.37	0.35	183.59	0.61	109.55
16	1052	METHYL ETHYL KETONE*	0.25	299.18	0.35	275.71	0.63	154.97	0.34	278.63	0.60	168.69
17	1303	n-PROPYL FORMATE	0.24	326.68	0.34	302.99	0.62	171.98	0.33	305.60	0.59	186.35

* Fluid is toxic. Special care needs to be taken in the selection of such fluids, if chosen for application.

18	1319	ISOPROPYL ACETATE*	0.23	456.90	0.33	428.11	0.61	251.67	0.32	430.66	0.58	270.39
19	1322	METHYL PROPIONATE	0.24	377.83	0.34	350.77	0.62	199.68	0.33	353.73	0.59	216.37
20	1427	METHYL tert-PENTYL ETHER*	0.21	331.17	0.31	313.93	0.60	205.72	0.31	315.01	0.58	217.39
21	1477	2,5-DIHYDROFURAN*	0.26	188.21	0.36	172.83	0.64	96.67	0.35	174.73	0.61	105.63
22	1521	CHLOROFORM*	0.26	148.42	0.36	137.84	0.64	77.06	0.35	139.30	0.61	84.15
23	1523	1,2-DICHLOROETHANE*	0.27	218.11	0.37	202.62	0.65	111.75	0.36	204.78	0.62	122.33
24	**1580**	**cis-1,2-DICHLOROETHYLENE***	**0.26**	**123.16**	**0.36**	**114.33**	**0.64**	**63.90**	**0.35**	**115.55**	**0.61**	**69.79**
25	**1681**	**METHYL IODIDE***	**0.26**	**98.07**	**0.36**	**91.19**	**0.64**	**50.88**	**0.35**	**92.15**	**0.61**	**55.57**
26	**1684**	**ISOPROPYL IODIDE**	**0.27**	**203.69**	**0.37**	**186.90**	**0.65**	**102.90**	**0.36**	**189.21**	**0.62**	**112.51**
27	1742	ETHYLENEIMINE*	0.26	166.17	0.36	154.22	0.64	86.25	0.35	155.87	0.61	94.20
28	1775	METHACRYLONITRILE*	0.26	258.18	0.36	236.89	0.64	132.12	0.35	239.43	0.61	144.37
29	1804	tert-BUTYL MERCAPTAN*	0.23	202.62	0.32	190.62	0.61	114.34	0.32	191.62	0.58	122.55
30	1805	ISOBUTYL MERCAPTAN	0.24	256.46	0.34	239.93	0.63	138.11	0.34	241.51	0.60	148.97
31	1806	sec-BUTYL MERCAPTAN	0.24	245.47	0.34	229.89	0.62	133.11	0.33	231.35	0.60	143.45
32	**1821**	**THIOPHENE***	**0.27**	**188.08**	**0.37**	**173.37**	**0.65**	**95.53**	**0.36**	**175.34**	**0.62**	**104.71**
33	2306	tert-BUTYL FORMATE	0.23	315.87	0.32	297.48	0.61	180.42	0.32	298.92	0.58	192.78
34	2526	1,1-DICHLOROPROPANE*	0.26	246.32	0.35	226.86	0.64	126.43	0.35	229.32	0.61	137.75
35	3968	GERMANIUM TETRACHLORIDE*	0.26	192.41	0.36	177.98	0.64	99.54	0.35	179.87	0.61	108.69

* Fluid is toxic. Special care needs to be taken in the selection of such fluids, if chosen for application.

Evaporation Temperature at 350 °C			POWER CYCLE		COMBINED HEAT AND POWER CYCLE							
					Thermal Utility Temperature = 40 °C				Thermal Utility Temperature = 80 °C			
					10% Q_{in}		40% Q_{in}		10% Q_{in}		40% Q_{in}	
S.No	**CHEM ID**	**Fluid Name**	**η**	**V_r**	**η**	**V_r**	**η**	**V_r**	**η**	**V_r**	**η**	**V_r**
1	274	CYCLOOCTENE*	0.26	4863.60	0.36	4598.91	0.64	2721.67	0.35	4618.58	0.62	2896.84
2	292	PROPENYL CYCLOHEXENE*	0.25	6919.98	0.35	6554.94	0.64	4021.89	0.35	6580.15	0.62	4260.73
3	333	1,5-CYCLOOCTADIENE*	0.27	4755.26	0.37	4486.83	0.65	2562.10	0.36	4509.01	0.63	2745.54
4	505	o-XYLENE*	0.28	4607.11	0.38	4334.33	0.66	2396.84	0.37	4359.58	0.63	2587.68
5	509	n-PROPYLBENZENE	0.27	6364.46	0.36	6012.63	0.65	3514.91	0.36	6040.14	0.63	3753.99
6	513	p-ETHYLTOLUENE	0.27	7148.04	0.37	6745.27	0.66	3857.71	0.37	6778.60	0.63	4135.34
7	601	STYRENE*	0.29	4168.47	0.38	3907.32	0.67	2089.72	0.38	3934.23	0.64	2269.94
8	**615**	**ETHYNYLBENZENE***	**0.29**	**2918.52**	**0.39**	**2731.16**	**0.67**	**1441.10**	**0.38**	**2751.48**	**0.64**	**1569.76**
9	1508	1,4-DICHLOROBUTANE	0.30	5729.95	0.39	5314.19	0.68	2751.75	0.39	5367.34	0.65	3019.80
10	**1721**	**PYRROLE**	**0.32**	**3363.38**	**0.42**	**3146.66**	**0.70**	**1613.98**	**0.41**	**3181.19**	**0.67**	**1790.60**
11	1811	CYCLOHEXYL MERCAPTAN	0.28	4160.15	0.38	3922.63	0.66	2168.72	0.37	3943.35	0.64	2334.01
12	**1843**	**TETRAHYDROTHIOPHENE**	**0.30**	**2008.30**	**0.40**	**1857.05**	**0.68**	**952.87**	**0.39**	**1877.86**	**0.65**	**1049.01**
13	2797	3-METHYLPYRIDINE*	0.31	3879.59	0.40	3589.81	0.69	1819.43	0.40	3629.53	0.66	2004.82
14	2799	4-METHYLPYRIDINE*	0.31	3951.26	0.40	3654.76	0.69	1850.28	0.40	3695.67	0.66	2039.47
15	**3927**	**ARSENIC (III) CHLORIDE***	**0.31**	**2623.92**	**0.41**	**2452.52**	**0.69**	**1277.61**	**0.40**	**2477.01**	**0.66**	**1411.02**

* Fluid is toxic. Special care needs to be taken in the selection of such fluids, if chosen for application.

ANNEX 2: Efficiency versus Size Parameter plots

At T_h = 150 °C

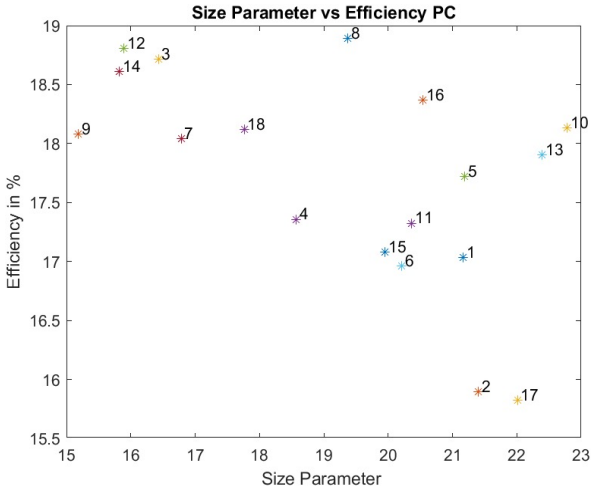

Figure 7: Results for power cycle

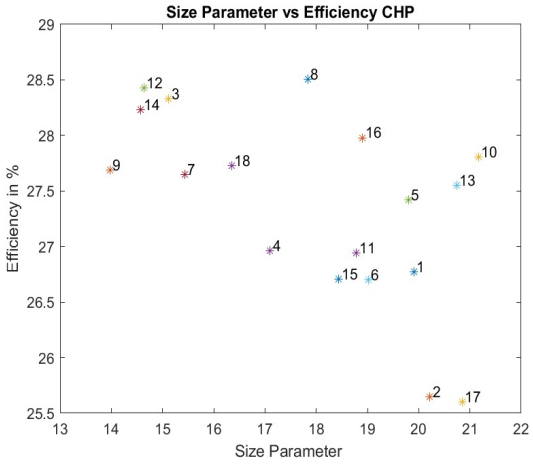

Figure 8: Results for CHP, f=0.1, T_u=40°C

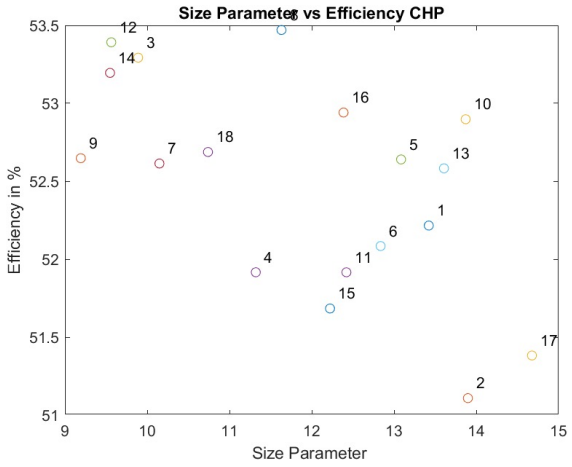

Figure 9: Results for CHP, f=0.4, T_u=40°C

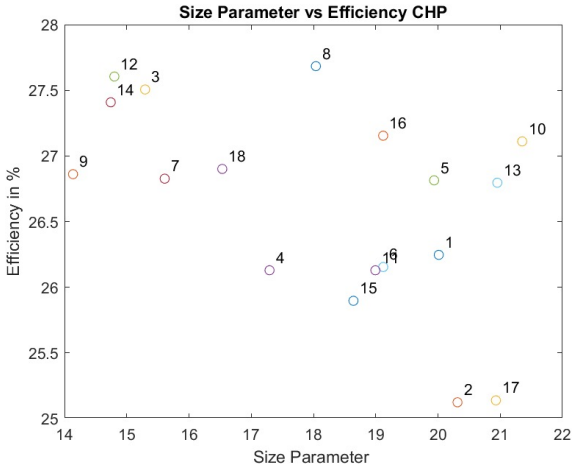

Figure 10: Results for CHP, f=0.1, T_u=80°C

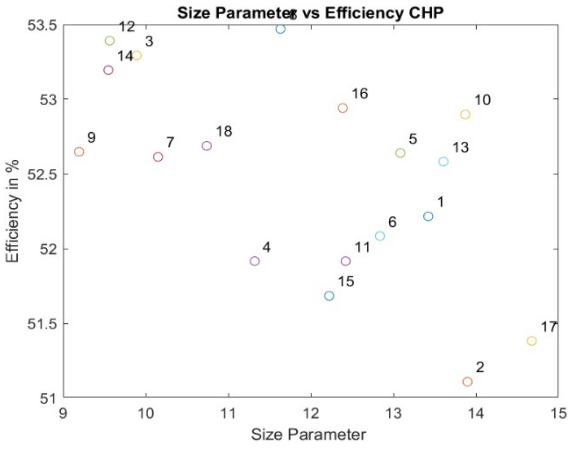

Figure 11: Results for CHP, f=0.4, T_u=80°C

At T_h = 250 ℃

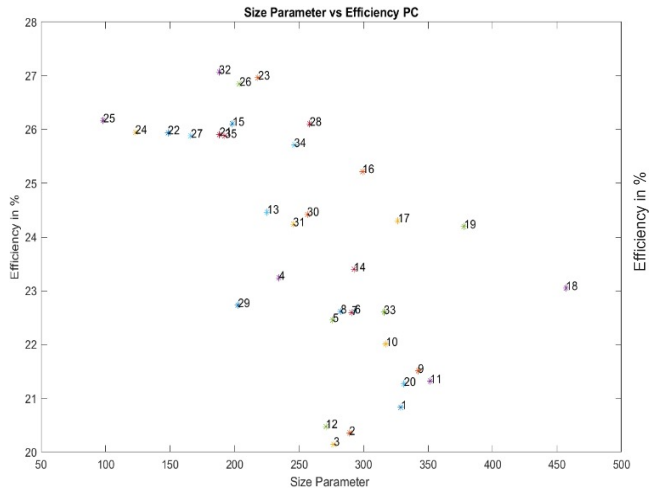

Figure 12: Results for power cycle

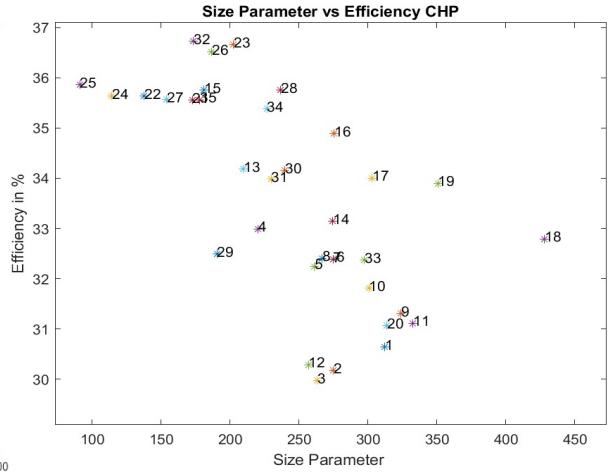

Figure 13: Results for CHP, f=0.1, T_u=40℃

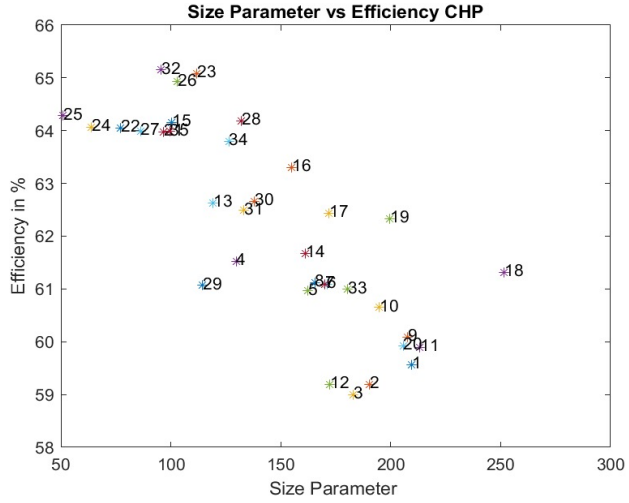

Figure 14: Results for CHP, f=0.4, T_u=40℃

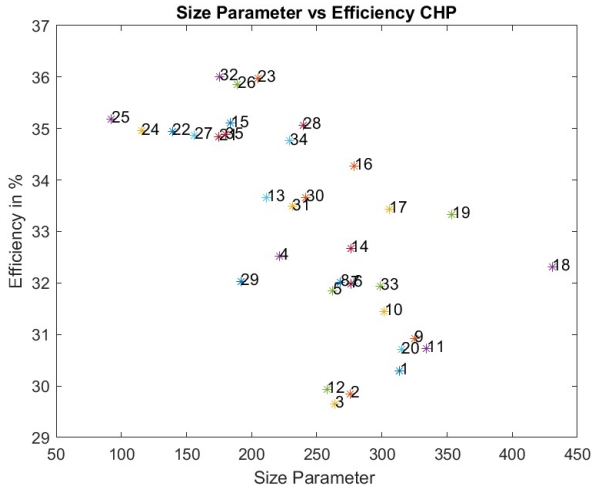

Figure 15: Results for CHP, f=0.1, T_u=80℃

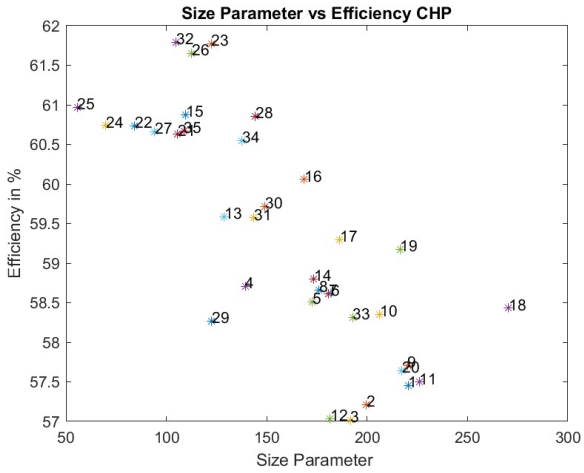

Figure 16: Results for CHP, f=0.4, T_u=80℃

At T_h = 350 ℃

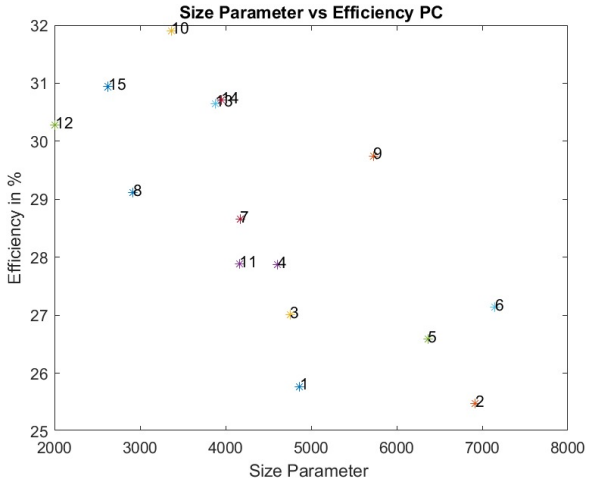

Figure 17: Results for Power cycle

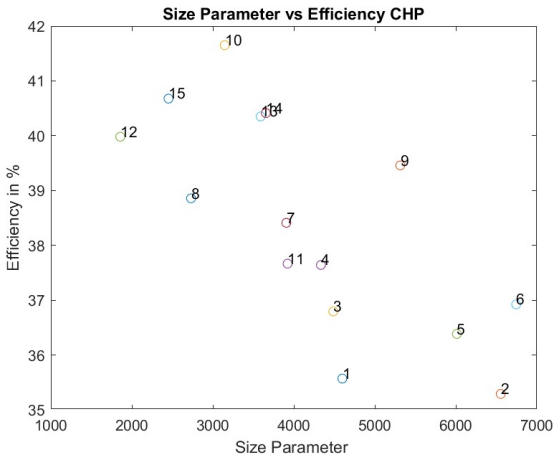

Figure 18: Results for CHP, f=0.1, T_u=40℃

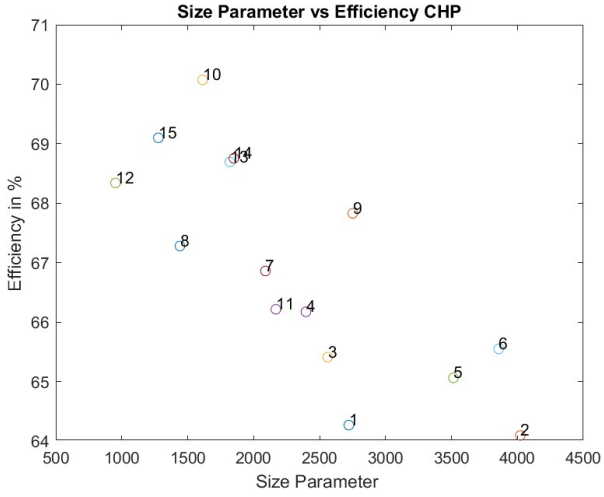

Figure 19: Results for CHP, f=0.4, T_u=40℃

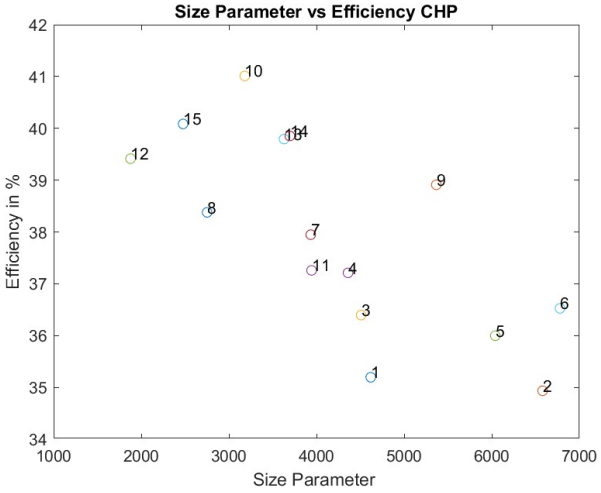

Figure 20: Results for CHP, f=0.1, T_u=80℃

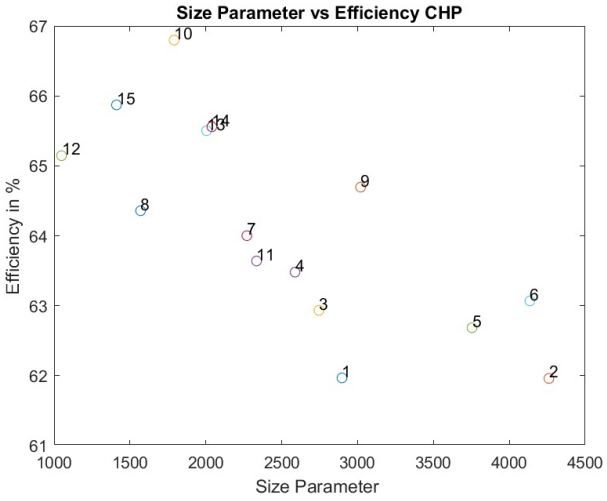

Figure 21: Results for CHP, f=0.4, T_u=80℃

ANNEX 3: Document for the execution of the MATLAB program *thermtry.m*

The code is written in MATLAB® R2021a, hence compatibility with previous versions must be ensured. The program uses the function "ThermeProp" which is an independent program required to be installed in the same directory as MATLAB for the execution of this program. Separate documentation on "ThermeProp" is available.

The list of steps are as follows:

1. Import the "*Fluides.dat*" folder in MATLAB before executing the code. This file must be saved in the same directory as MATLAB.
2. Run the program.
3. It asks the user to select files to screen the fluid. In this case, all 647 fluids in our database are selected.
4. The user is then asked to provide the inputs in sequence as:
   a. *Insert the source temperature in Celsius*: The user needs to provide the source temperature/evaporator temperature mainly in this case: **150, 250 or 350.**
   b. *Insert the percentage of heat used for thermal utility*: The user needs to input values in decimal, in this case either **0.1 or 0.4**. However, if the user wants the results of the power cycle only, this value can be kept as 0.
   c. *Insert the thermal utility temperature in Celsius*: The user needs to input the temperature at which the heat is required to be extracted for heating in the CHP. In our study, this value was **40 or 80.** For power cycle only, this value can also be kept as 0.
5. After execution of the program, three figures are displayed:
   a. **Figure 1**: A scatter plot of *Size Parameter* vs *Efficiency* of all the filtered fluids for the power cycle. The filtered fluids are numbered in the plot. The Size Parameter is plotted in the *x*-axis and Efficiency in the *y*-axis.
   b. **Figure 2**: A scatter plot of *Size Parameter* vs *Efficiency* of all the filtered fluids for the CHP. The filtered fluids are numbered in the plot. The *x*-axis and *y*-axis are the same as in the previous figure.
   c. **Figure 3**: A scatter plot of *Size Parameter* vs *Efficiency* of all the filtered fluids for the power as well as CHP cycle. The filtered fluids are numbered as earlier, and the axes are the same. This is a single plot containing both the above plots. It shows the changes in the performance of the fluids in the power and CHP cycles.
6. In the list of output variables, **Result** can be seen which is a multi-dimensional table with:
   a. *Column 1*: Contains the number of fluids obtained after the screening process.
   b. *Column 2*: Contains the ChemID of the corresponding fluids – this is same as the ChemID in the parent file "*Fluides.dat*" which has been described in the "*ThermeProp*" document.
   c. *Column 3*: Contains the chemical name of the fluids obtained after the screening process.
7. **V_r and V_R**: Contains the values of the size parameters for power and CHP cycles respectively.
8. **eff and EFF**: Contains the list of efficiencies (as a percentage) of the filtered fluids for power and CHP cycles respectively.

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MATLAB CODE

READING FLUIDES FILES

```
[file_list]=uigetfile('.fld','Fluid Files','Multiselect','on'); %"
 this function allows to import files"
```

- DEFINITION OF VARIABLES*

```
%ts = 350;  % temperature of Hot source
 tamb = 20 ; % Ambient Temperature
 tpinch = 10; % Pinch point temperature
% hin = 0.4;
% Tu = 80;
 ts = input('Insert the source temperature in Celcius ');
 hin = input('Insert the percentage of heat to be used as thermal
 utility: ');
 Tu = input('Insert the thermal utility temperature in Celcius ');

 tcr = ts + 5.00 ; % Critical Temperature Sorting of the fluids
 ttp = tamb ; % Triple point temperature for sorting of the fluids
 ambient temp
 tc = 273.15 + tamb + tpinch ;  % temperature at the exit of the
 turbine amb temp + pinch point
 th = 273.15 + ts ; % temperature at the inlet of the turbine

if ts == 150
    PH = 35; % critical pressure assumption of Psat @ TH
    PC = 1;  %condensor pressure assumption to be made of Psat at Tc
+10
end
if ts == 250
    PH = 70;
    PC = 0.1;
end
if ts == 350
    PH = 150;
    PC = 0.005;
end

 Dc = 0.01 ; % Density of fluid @Tc and Pc
 GWP = 150 ; % Global warming Potential
 ODP = num2str('NO');  % Consideration for Bromine only
 AITC = ts/0.8 ; % Ignition Temperature

 Peff = 1 ; % Efficiency of pump
 Teff = 0.85; % Efficiency of Turbine


 C1 = 0 ; C2 = 0; C3 = 0; C4 = 0; C5=0; C6=0; C7 = 0; C8 = 0;  %
 Counter for filter Tcr,Ttp & Psat @Tc

Chemid=Fluides.Chemid;
```

```
TC= Fluides.TCC;
Name=Fluides.Name;
TTP = Fluides.TPTC;
Global=Fluides.GWP;
Ozone=Fluides.BromineNOabsentXpresent;
Ignition=Fluides.AITC;
F1 = zeros(1,1);     N1 = strings(1,1);
F2 = zeros(1,1);     N2 = strings(1,1);
F3 = zeros(1,1);     N3 = strings(1,1);
F4 = zeros(1,1);     N4 = strings(1,1);
F5 = zeros(1,1);     N5 = strings(1,1);
F6 = zeros(1,1);     N6 = strings(1,1);
F7 = zeros(1,1);     N7 = strings(1,1);
F8 = zeros(1,1);     N8 = strings(1,1);
P = zeros(1,1);      A= zeros(1,1);     G1 = zeros(1,1);
I1 = zeros(1,1);      tf = zeros(1,1);   O1 = strings(1,1);
P2= zeros(1,1);       Den = zeros(1,1);
Chem2 = zeros(1,1);   Chem3 = zeros(1,1);   Chem4 = zeros(1,1);
Chem5 = zeros(1,1);   Chem6 = zeros(1,1);   Chem7 = zeros(1,1);
Chem8 = zeros(1,1);

S1 = zeros(1,1);    P1 = zeros(1,1);   H1 = zeros(1,1);
H2S = zeros(1,1);   H2 = zeros(1,1);   H5S = zeros(1,1);
H4 = zeros(1,1);    S4 = zeros(1,1);   H5 = zeros(1,1);
P3 = zeros(1,1);    H3 = zeros(1,1);    WT= zeros(1,1);
WP= zeros(1,1);   Eff= zeros(1,1);
Qin = zeros(1,1);

p5s = zeros(1,1);  h5s = zeros(1,1); h5 = zeros(1,1);
h6 = zeros(1,1);   x6 = zeros(1,1);  s6 = zeros(1,1);
h7s = zeros(1,1);  h7 = zeros(1,1); x7 = zeros(1,1);
qin= zeros(1,1);   wt = zeros(1,1);  eff = zeros(1,1);
```

SCREENING OF FLUIDS

```
for i=1:1:647
if TC(i) >= tcr %sorting for consideration with Critical Point
 Temperature
    C1=C1+1;
    F1(C1,1) = TC(i,1);
    N1(C1,1)=Name(i,1);

         if TTP(i) <= ttp  % sorting for consideration with Triple
 Point Temperature
         C2=C2+1;
         F2(C2,1)=TTP(i,1);
         N2(C2,1)=Name(i,1);
         Chem2(C2,1)=Chemid(i,1);
         P(C2,1) = thermepropm('P','T',tc,'Q',0,Chem2(C2));

          if P(C2) >= PC         % sorting for consideration with Psat
 @Tc
            C3= C3+1;
            F3(C3,1)=P(C2,1);
```

```
            N3(C3,1)=Name(i,1);
          Chem3(C3,1)=Chemid(i,1);

          A(C3,1) = thermepropm('P','T',th,'Q',0,Chem3(C3));
        if A(C3) <= PH         % sorting for consideration with Psat
@TH
            C4= C4+1;
            F4(C4,1)=A(C3,1);
            N4(C4,1)=Name(i,1);
            Chem4(C4,1)=Chemid(i,1);

          P2(C4,1) = thermepropm('P','T',tc,'Q',0,Chem4(C4));
          Den(C4,1) = thermepropm('D','T',tc,'P',P2(C4,1),Chem4(C4));
        if Den(C4,1)>= Dc    % sorting for consideration with Density
@ Tc
            C5= C5+1;
            F5(C5,1)=Den(C4,1);
            N5(C5,1)=Name(i,1);
            Chem5(C5,1)=Chemid(i,1);

            G1(C5,1) = Global(i,1);
         if G1(C5,1) < 150     % sorting for consideration with GWP
            C6 = C6 + 1;
            F6(C6,1)=G1(C5,1);
            N6(C6,1)=Name(i,1);
            Chem6(C6,1)=Chemid(i,1);

         O1(C6,1) = Ozone(i,1);
          tf(C6,1) = strcmp(O1(C6,1),ODP);
         if  tf(C6,1) == 1    % sorting for consideration with ODP
            C7 = C7 + 1;
            F7(C7,1)=O1(C6,1);
            N7(C7,1)=Name(i,1);
            Chem7(C7,1)=Chemid(i,1);

            I1(C7,1) = Ignition(i,1);
         if I1(C7,1) > AITC    % sorting for consideration with AITC

            C8 = C8 + 1;
            F8(C8,1)=I1(C7,1);
            N8(C8,1)=Name(i,1);
            Chem8(C8,1)=Chemid(i,1);

           %Creating a single table
           Result(C8,:) =
 table(C8,Chem8(C8,1),N8(C8,1),'VariableNames',
{'S.No','ChemID','Name'});
```

RANKINE CYCLE

```
           % Point 1
            S1(C8,1) =  thermepropm('S','T',tc,'Q',0,Chem8(C8));    %
 Entropy at point 1
            P1(C8,1) =  thermepropm('P','T',tc,'Q',0,Chem8(C8));
  % Saturation Pressure at point 1
```

```
            H1(C8,1) = thermepropm('H','T',tc,'Q',0,Chem8(C8));     %
 Enthalpy at point 1
            % Point 3
            P3(C8,1) =  thermepropm('P','T',ts
+273.15,'Q',0,Chem8(C8));     % Pressure at point 3
           % H3(C8,1) =  thermepropm('H','T',ts
+273.15,'Q',0,Chem8(C8));     % Pressure at point 3
            % Point 2S
            H2S(C8,1) =
 thermepropm('H','P',P3(C8,1),'S',S1(C8,1),Chem8(C8)); % Enthalpy at
 point 2S
            H2(C8,1) = H1(C8,1) + (H2S(C8,1) - H1(C8,1))/Peff;
  %Enthalpy at point 2
            % Point 4
            H4(C8,1) = thermepropm('H','T',ts
+273.15,'Q',1,Chem8(C8));  % Enthalpy at point 4
            S4(C8,1) =  thermepropm('S','T',ts
+273.15,'Q',1,Chem8(C8));    % Entropy at point 4
            D4(C8,1) = thermepropm('D','T',ts
+273.15,'Q',1,Chem8(C8));   % Density of fluid at inlet of turbine
 point 4
            V4(C8,1) = 1/D4(C8,1) ; % Volume at point 4
            % Point 5S
            H5S(C8,1) =
 thermepropm('H','P',P1(C8,1),'S',S4(C8,1),Chem8(C8)); % Enthalpy at
 point 5S
            X5S(C8,1) =
 thermepropm('Q','P',P1(C8,1),'S',S4(C8,1),Chem8(C8));    % Quality of
 vapor at the exit of turbine
            D5S(C8,1) =
 thermepropm('D','P',P1(C8,1),'S',S4(C8,1),Chem8(C8)); %Density of
 fluid at outlet of turbine
            V5S(C8,1) = 1/D5S(C8,1); % Specific volume ta point 5s
            % Point 5
            H5(C8,1) = H4(C8,1) - Teff * (H4(C8,1)-H5S(C8,1));
  %Enthalpy at point 5
            D5(C8,1) =
 thermepropm('D','P',P1(C8,1),'S',S4(C8,1),Chem8(C8)); %Density of
 fluid at outlet of turbine
            V5(C8,1) = 1/D5(C8,1); % Specific volume ta point 5
            WP(C8,1) = (H2(C8,1)-H1(C8,1));                      %
 Work input Pump
            WT(C8,1) = (H4(C8,1)-H5(C8,1));                      %
 Turbine Work Out
            Qin(C8,1) = (H4(C8,1)-H2(C8,1));                     %
 Work input
            Eff(C8,1) = ((H4(C8,1)-H5(C8,1))-(H2(C8,1)-H1(C8,1)))/
(H4(C8,1)-H2(C8,1));  % Efficiency

             % Size Parameter
             SP(C8,1) = ((V5S(C8,1))^0.5)/((H4(C8,1)-
H5S(C8,1))^0.25);  % Size parameter of the fluids
             Vr(C8,1) = V5(C8,1)/V4(C8,1);  % Relative volume ratio
 turbine
```

```
            % Intermediate calculation
          Qreq = 0.6;         % Acceptable vapor quality at the
turbine inlet/outl
          % Tu = 40;
          tuT = Tu + 273.15;  % Thermal utility temeperature
          t6 = tuT + tpinch;  % Saturation Temperature at
intermediate pressure
          p5s(C8,1) = thermepropm('P','T',t6,'Q',1,Chem8(C8)); %
Intermediate pressure
          h5s(C8,1) =
thermepropm('H','P',p5s(C8,1),'S',S4(C8,1),Chem8(C8)); % Enthalpy at
point 5S
          h5(C8,1) = H4(C8,1) - Teff * (H4(C8,1)- h5s(C8,1));
 %Enthalpy at point 5

          % Taking percentage of Heat Input
          % hin = 0.1 ;     % percentage of heat to be used of the
input heat
          qin(C8,1) = hin * Qin(C8,1);  % Heat that is being used
          h6(C8,1) = h5(C8,1) - qin(C8,1); % Enthalpy at the inlet
of second turbine
          s6(C8,1) =
thermepropm('S','P',p5s(C8,1),'H',h6(C8,1),Chem8(C8));    % Entropy
at point 6
          x6(C8,1) =
thermepropm('Q','P',p5s(C8,1),'H',h6(C8,1),Chem8(C8));    % Quality
of vapor at 2nd turbine inlet point 6

          % Point 7s
          h7s(C8,1) =
thermepropm('H','P',P1(C8,1),'S',s6(C8,1),Chem8(C8)); % Enthalpy at
point 7s exit of 2nd turbine (ideal)
          h7(C8,1) =  h6(C8,1) - Teff * (h6(C8,1)- h7s(C8,1));
      % Enthalpy at point 7 at exit of turbine
          x7(C8,1) =
thermepropm('Q','P',P1(C8,1),'H',h7(C8,1),Chem8(C8));  % Quality of
vapor at 2nd turbine exit point 6
          d7(C8,1) =
thermepropm('D','P',P1(C8,1),'H',h7(C8,1),Chem8(C8)); %Density of
fluid at outlet of 2nd turbine
          v7(C8,1) = 1/d7(C8,1); % Specific volume at point 7
          wt(C8,1) = H4(C8,1) - h5(C8,1) + h6(C8,1) - h7(C8,1); %
Total work output of CHP
          eff(C8,1) = (wt(C8,1)+qin(C8,1)-WP(C8,1))/Qin(C8,1) ;
 % Combined Efficiency of the Cycle

          % Size Parameter
         VR(C8,1) = v7(C8,1)/V4(C8,1);  % Relative volume ratio
turbine
         %Figure plots
         figure(1)
            plot(Vr(C8,1),Eff(C8,1)*100,'*');
```

```
                text(Vr(C8,1)+0.05,Eff(C8,1)*100+0.05,num2str(C8));
                title('Size Parameter vs Efficiency PC')
                xlabel('Size Parameter ')
                ylabel('Efficiency in %')
                grid off
                hold on

                figure(2)
                plot(VR(C8,1),eff(C8,1)*100,'o');
                text(VR(C8,1)+0.1,eff(C8,1)*100+0.1,num2str(C8));
                title('Size Parameter vs Efficiency CHP')
                xlabel('Size Parameter ')
                ylabel('Efficiency in %')
                grid off
                hold on

                figure(3)

 plot(VR(C8,1),Eff(C8,1)*100,'*',VR(C8,1),eff(C8,1)*100,'o','Linewidth',1.5,'color
                  text(VR(C8,1)+0.05,Eff(C8,1)*100+0.05,num2str(C8));
                  text(VR(C8,1)+0.05,eff(C8,1)*100+0.05,num2str(C8));
                  title('Fluids vs Efficiency in PC & CHP')
                  xlabel('Size Parameter')
                  ylabel('Efficiency in %')
                  legend( 'Power Cycle','Combined Heat Power Cycle')
                  grid off
                  hold on

            else
               end
            else
              end
            else
              end
           else
              end
           else
              end
            else
              end
           else
               end
else
                  end
end
```

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